Introduction to Geometric Mechanics and AVI

François Demoures

Tudor Ratiu, Yves Weinand

CAG, IBOIS, EPFL

francois.demoures@epfl.ch

MIT - Prof Radovitzky, May 13, 2010

Plan of presentation

- Continuous mechanics
- Discrete mechanics
- Asynchronous Variational Integrator

Continuous mechanics

References for continuous mechanics

Ralph Abraham, Jerrold E. Marsden [1987], Foundations of Mechanics. *Addison-Wesley Publishing Company, Inc.*

Ralph Abraham, Jerrold E. Marsden, Tudor S. Ratiu [1991], Manifolds, Tensor Analysis, and Applications. *Springer*

Jerrold E. Marsden, Tudor S. Ratiu [1999], Introduction to Mechanics and Symmetry. *Springer*

Continuous mechanics

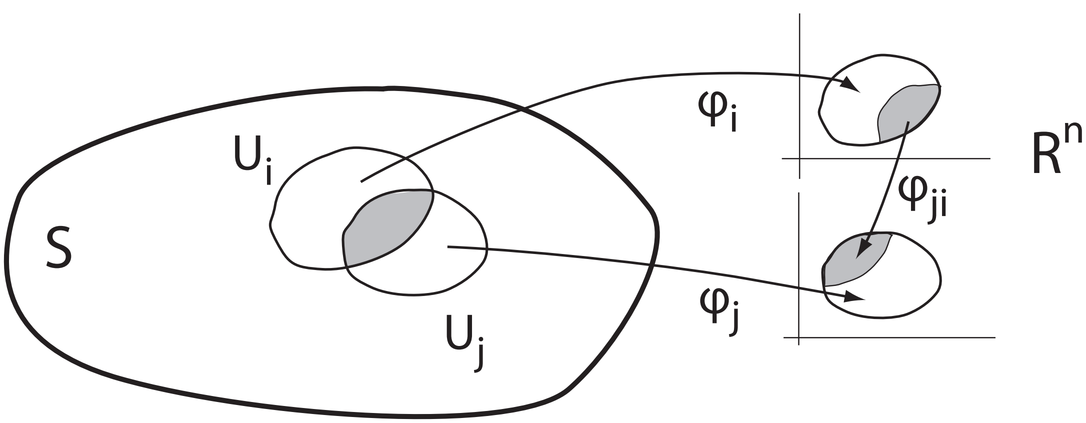
- a) Differentiable manifold and tangent bundle
- b) Lagrangian mechanics
- c) Hamiltonian mechanics
- d) Lie group and Lie algebra
- e) Symplectic property and Noether's theorem

Differentiable manifold. The basic idea of a manifold is to introduce a local object that will support differentiation process.

Let S a set, and $U \subset S$ with a one-to-one mapping $\phi : U \to F$ as a **chart** (U, ϕ) or **coordinate system** $\{x^i\}$, where x^i denote the components of this mapping. Where F is a subset of a Banach space, as $\mathbb{R}^n$.

For two charts (U_i, ϕ_i), (U_j, ϕ_j) and $\phi_i \cap \phi_j \neq \emptyset$ let the **overlap map** $\phi_{ji} = \phi_j \circ \phi_i^{-1} : \phi_i(U_i \cap U_j) \to \phi_j(U_i \cap U_j)$.

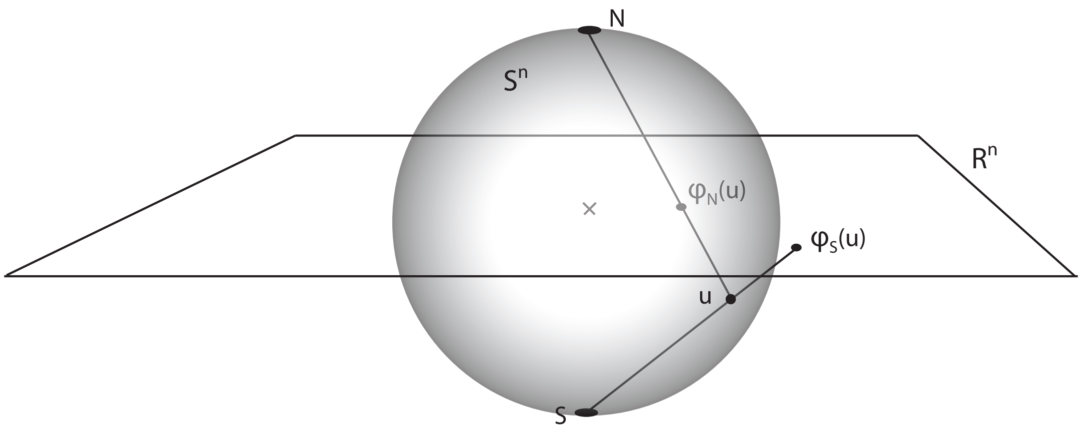
An **atlas** $\mathcal{A}$ on S is a family of charts such that $S = \bigcup_{i \in I} U_i$, and overlap maps ϕ_{ji} are C^∞ diffeomorphisms.



S is a **differentiable manifold**, or a C^k-**manifold**, if S is covered by a collection of charts $\{(U_i, \phi_i)\}$, and if S has an atlas $\mathcal{A}$. (If a chart is compatible with a given atlas, then it can be included into the atlas itself to produce a larger atlas.)

Example :

In $\mathbb{R}^n$ consider the n-sphere S^n. Let the atlas $\mathcal{A}$ composed of two charts (U_N, ϕ_N) and (U_S, ϕ_S), where $U_N = S^n \setminus \{N\}$, $U_S = S^n \setminus \{S\}$.



with overlap maps

$$\phi_S \circ \phi_N^{-1}(x) = \frac{1}{\|x\|^2}\, x, \quad \phi_N \circ \phi_S^{-1}(y) = \frac{1}{\|y\|^2}\, y, \quad x, y \in \mathbb{R}^n \setminus \{0\}$$

Tangent bundle.

Let M a differentiable n-manifold with local coordinate $\{x^i\}$, the **tangent bundle** of M, denoted by TM, is the set of the tangent space to M at the points $m \in M$, that is

$$TM = \bigcup_{m \in M} T_m M.$$

TM is a 2n-manifold, with local coordinate $\{x^i, v^i\}$, where $\{v^i\}$ is a tangent vector.

The **natural projection** is the map

$$\tau_M : TM \longrightarrow M, \quad v \mapsto m$$

where v is the vector attached to the point m. And the inverse image $\tau_M^{-1}(m)$ is the **fiber** of the tangent bundle over the point $m \in M$.

Lagrangian mechanics.

Configuration space Q as a manifold, is the *set of all possible spatial positions of bodies in the system*. Given a time interval $[0, T]$ define the **path space** to be $\mathcal{C}(Q) = \{q : [0, T] \to Q \mid q \in C^2([0, T])\}$, which is a C^∞-manifold.

The collection of pairs $(q, \dot{q})$ as elements of the tangent bundle $T_q Q$, also called **velocity phase space**, with basis $\{\partial/\partial q^1, ..., \partial/\partial q^n\}$.

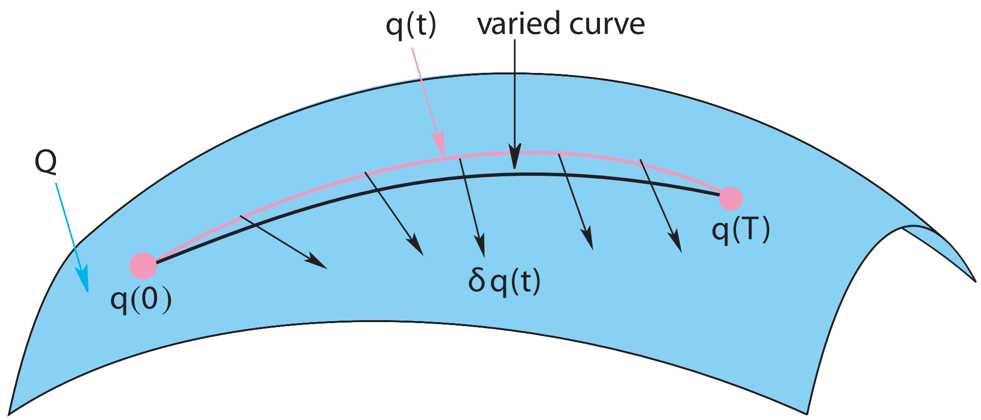
The **Lagrangian** $L(q^i, \dot{q}^i) : TQ \to \mathbb{R}$ is often seen as the kinetic energy minus the potential energy, where $(q^1, ..., q^n)$ are configurations coordinates.

Given a time interval $[0, T]$, let the **action map** $\mathfrak{G} : \mathcal{C}(Q) \to \mathbb{R}$

$$\mathfrak{G}(q) = \int_0^T L(q^i(t), \dot{q}^i(t))dt.$$

Hamilton's principle or **principle of critical action**, seeks curves $q(t)$ for which the **action map** $\mathfrak{G}$ is stationary under variations of $q(t)$ with fixed endpoints : $\delta q^i(0) = \delta q^i(T) = 0$, and time interval.

$$\delta\mathfrak{G}(q) = \int_0^T \left(\frac{\partial L}{\partial q^i}\delta q^i + \frac{\partial L}{\partial \dot{q}^i}\delta \dot{q}^i \right) dt = \int_0^T \left(\frac{\partial L}{\partial q^i}\delta q^i - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}^i}\delta q^i \right) dt = 0$$



gives the well-known **Euler-Lagrange equations** :

$$\frac{\partial L}{\partial q^i} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}^i} = 0$$

Example : For a system of N particles* moving in Euclidean 3-space, we choose the configuration space to be $Q = \mathbb{R}^3 \times ... \times \mathbb{R}^3 = \mathbb{R}^{3N}$, and

$$L(\mathbf{q}_j, \dot{\mathbf{q}}_j) = \frac{1}{2} \sum_{j=1}^{N} m_j \|\dot{\mathbf{q}}_j\|^2 - V(\mathbf{q}_j), \quad \mathbf{q}_j \in \mathbb{R}^3$$

Where $\frac{1}{2} m_j ||\dot{\mathbf{q}}_j||^2$ is the kinetic energy, and $V(\mathbf{q}_j)$ is the potential energy of the particle j.

The Euler-Lagrange equations are

$$\frac{d}{dt}\Big(m_j \dot{q}_j\Big) = -\frac{\partial V}{\partial q_j}, \quad j = 1, ..., N. \quad \square$$

*__Newton's second law__ for a particle $\mathbf{q}_j$ moving in Euclidean three-space $\mathbb{R}^3$ under the influence of a potential energy $V(\mathbf{q}_j)$ is : $m\ddot{\mathbf{q}}_j = -\nabla V(\mathbf{q_j})$

Hamiltonian mechanics.

Motivation : For a particle $\mathbf{q}$, let E the **total energy**, such that $dE/dt = 0$, as

$$E(\mathbf{q}) = \frac{1}{2}m||\dot{q}||^2 + V(q)$$

Lagrange and Hamilton observed that it is convenient to introduce the momentum $p_i = m\dot{q}^i$ and rewrite E as

$$H(\mathbf{q}, \mathbf{p}) = \frac{||\dot{\mathbf{p}}||^2}{2m} + V(\mathbf{q})$$

for then Newton's second law is equivalent to **Hamilton's canonical equations**

$$\dot{q}^i = \frac{\partial H}{\partial p_i}, \quad \dot{p}_i = -\frac{\partial H}{\partial q^i}$$

where $(\mathbf{q}, \mathbf{p})$ is **phase space**. $\square$

Let a manifold M, the **cotangent bundle** T^*M, or the dual of TM, is the space of differential $\mathbf{d}f$, for all smooth function $f : M \to \mathbb{R}$.

$$\mathbf{d}f(x) = \frac{\partial f}{\partial x^i} dx^i$$

The cotangent bundle T^*Q of the configuration space Q is the space where $(dq^1, ..., dq^n)$.

Define the **fiber derivative** or **Legendre transform** $\mathbb{F}L : TQ \to T^*Q$ by

$$\mathbb{F}L(v).w = \frac{d}{ds}\bigg|_{s=0} L(v + sw), \qquad v, w \in T_qQ$$

which is the derivative of Lagrangian L at v along the fiber T_qQ in the direction w. So, for finite-dimensional manifold and $(q^i, \dot{q}^i)$ coordinates on T_qQ, we get

$$\mathbb{F}L(q^i, \dot{q}^i) = \left(q^i, \frac{\partial L}{\partial \dot{q}^i} \right) = (q^i, p_i) \in T_q^*Q,$$

where p_i is the **conjugate momenta** which is not always $m\dot{\mathbf{q}}$.

If the fiber derivative $\mathbb{F}L$ is locally an isomorphism then we say that L is **regular**.

Assume that Legendre transform is invertible and define the **Hamiltonian** $H : T^*Q \to \mathbb{R}$ by

$$H(q^i, p_i) = p_i \dot{q}^i - L(q^i, \dot{q}^i),$$

then the Euler-Lagrange equations are equivalent to **Hamilton's equations**

$$\dot{q}^i = \frac{\partial H}{\partial p_i}, \quad \dot{p}_i = -\frac{\partial H}{\partial q_i}, \quad i = 1, ..., n.$$

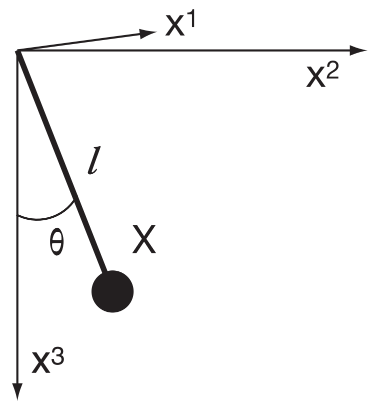
Which can be view as follows

$$\left(\frac{\partial H}{\partial p_i}, -\frac{\partial H}{\partial q^i} \right) = (\dot{q^i}, \dot{p}_i)$$

$$\text{where} \quad X_H(z) =: \left(\frac{\partial H}{\partial p_i}, -\frac{\partial H}{\partial q^i} \right) = \begin{bmatrix} 0 & \mathrm{I} \\ -\mathrm{I} & 0 \end{bmatrix} \mathbf{d}H(z)$$

is the **Hamiltonian vector field**, and $(\mathbf{q}(t), \mathbf{p}(t))$ is an integral curve of X_H.

Example : simple pendulum. Lagrangian and Hamiltonian point of view.



The configuration space is the sphere S_l^2 of radii l

$$Q = S_l^2, \quad \begin{cases} x^1 = 0 \\ x^2 = l sin(\theta) \\ x^3 = l cos(\theta) \end{cases} \quad \begin{cases} \dot{x}^1 = 0 \\ \dot{x}^2 = \ \ l\dot{\theta} cos(\theta) \\ \dot{x}^3 = -l\dot{\theta} sin(\theta) \end{cases}$$

And, for Euclidean metric tensor g_{ij}, the Lagrangian $L(\theta, \dot{\theta})$ is

$$L(\theta, \dot{\theta}) = \frac{1}{2} m \sum_{i,j=1}^{3} g_{ij} \dot{x}^i \dot{x}^j - V(\theta) = \frac{1}{2} m \left(l\dot{\theta} \right)^2 + mg \left(l cos(\theta) \right)$$

Euler-Lagrange equation gives the **equation of the motion**

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{\theta}} \right) - \frac{\partial L}{\partial \theta} = ml^2 \ddot{\theta} + mgl sin(\theta) = 0$$

The conjugate momenta p_θ and the Hamiltonian are

$$p_\theta = \frac{\partial L}{\partial \dot{\theta}} = ml^2\dot{\theta}, \qquad H(\theta, p_\theta) = p_\theta\dot{\theta} - L(\theta, \dot{\theta}) = \frac{p_\theta^2}{2ml^2} - mglcos(\theta)$$

Hamilton's equations give us

$$\dot{p}_\theta = -\frac{\partial H}{\partial \theta} = -mglsin(\theta)$$

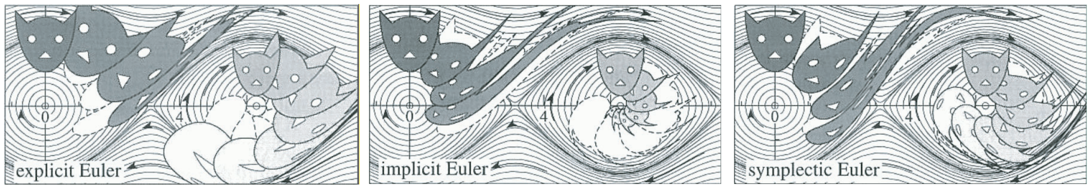
and, as previously, we get the **equation of the motion**

$$\dot{p}_\theta = \frac{d}{dt}(p_\theta) = ml^2\ddot{\theta} = -mglsin(\theta)$$

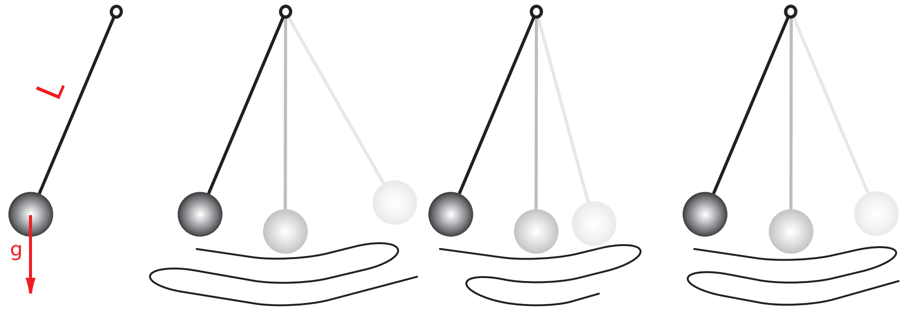
Remark : the Lagrangian L and the Hamiltonian H are invariant under rotation about the x^3 axis, as the symmetry group G for the pendulum. In such a way that we can consider the **reduce configuration space** $Q/G = S^1_l$, as the circle of radii l. $\square$

Symplectic property. Motivation :

Let a given region of initial conditions in phase-space $\{(q^i, p_i)\} \in T_q^*Q$. When the phenomenon is **symplectic**, if we advance all states simultaneously, regions of phase space, are deformed under the flow, in a way that preserves the original area, as on the right figure.



The *pendulum*: in this example three integrators behave very differently motion of a pendulum: while on the left it amplifies oscillations, and in the middle it dampens the motion, on the right the symplectic integrator captures the periodic nature of the pendulum.



$\square$

Let the **Hamiltonian vector field** $X_H : T^*Q \to T(T^*Q)$, as define $X_H(z) := \left(\frac{\partial H}{\partial p_i}, -\frac{\partial H}{\partial q^i}\right)$. And the **Hamiltonian flow** $F_H^t(z)$ which is the integral curve of $X_H(z)$.

Hamiltonian flows are symplectic. Formally, this means that the flow preserves the **canonical symplectic Hamiltonian two-form** $\Omega_H = \mathbf{d}q^i \wedge \mathbf{d}p_i$. Which means $F_H^* \Omega_H = \Omega_H$.

In the same way **Lagrangian flows** F_L^t **(i.e., motions) are symplectic**. Such as, if the Lagrangian is regular we can define F_L locally, as

$$F_L = \mathbb{F}L^{-1} \circ F_H \circ \mathbb{F}L.$$

Remark : The symplectic form $\Omega_H = \mathbf{d}q^i \wedge \mathbf{d}p_i$ defines the geometry of a symplectic manifold (T^*Q, Ω_H), much as the metric tensor defines the geometry of a Riemannian manifold.

Lie group and Lie algebra.

A **Lie group** is a manifold G that has a group structure (G, μ) consistent with its manifold structure in the sense that group operation

$$\mu : G \times G \to G, \quad (g, h) \mapsto \mu(g, h)$$

is a C^∞ map.

Examples : a) Any *Banach space* F, admits an atlas formed by the single chart identity, and is an Abelian Lie group with $+$ operation. We call such a group a **vector group**. (For example, the space $L(\mathbb{R}^n, \mathbb{R}^n)$ of all continuous linear maps of $\mathbb{R}^n$ to $\mathbb{R}^n$ is a Banach space and a vector group.)

b) The *orthogonal group* $O(n) = \{A \in GL(n, \mathbb{R})| \ AA^T = 1\}$, as a closed Lie subgroup of the Lie group $GL(n, \mathbb{R})$ of linear isomorphisms of $\mathbb{R}^n$ to $\mathbb{R}^n$, is a Lie group with group operation $\mu(A, B) = A \circ B$. $\quad \square$

Let G a Lie group, the vector space T_eG, as tangent vector to G at the identity $e \in G$, with Lie algebra structure $(T_eG, +, \cdot\ , [\ ,\ ])$ is called the **Lie algebra** of G, and is denoted by $\mathfrak{g}$. Where $[\ ,\ ]$ is the Lie bracket in T_eG.

Examples : a) For a Banach space F, the Lie algebra is itself, with the trivial bracket $[v, w] = 0$ for all $v, w \in F$.

b) The Lie algebra of $GL(n, \mathbb{R})$ is $L(\mathbb{R}^n, \mathbb{R}^n)$, also denoted $\mathfrak{gl}(n)$, with the bracket

$$[\widehat{v}, \widehat{w}] = \widehat{v}\widehat{w} - \widehat{w}\widehat{v}$$

c) The Lie algebra $\mathfrak{so}(3)$ of the Lie group $SO(3)$ is

$$\mathfrak{so}(3) = \{\widehat{v} : \mathbb{R}^3 \to \mathbb{R}^3 |\ \widehat{v} + \widehat{v}^T = 0\}$$

with the same bracket as for $\mathfrak{gl}(n)$. $\square$

Example of Lie group and Lie algebra application : thin-shell model of Simo and Fox.*

Let the differentiable manifold

$$\mathcal{C} := \{(\varphi, \mathbf{t}) |\ \mathcal{A} \subset \mathbb{R}^2 \to \mathbb{R}^3 \times S^2\}$$

where $\mathcal{A}$ is an open set with smooth boundary $\partial\mathcal{A}$, and compact closure $\mathcal{A}$. Any *configuration of the shell* is assumed to be defined by a pair $(\varphi, \mathbf{t}) \in \mathcal{C}$ as

$$S := \{x \in \mathbb{R}^3 |\ x = \varphi + \xi \mathbf{t},\ \text{where } (\varphi, \mathbf{t}) \in C,\ \xi \in \left[h^-, h^+\right]\}$$

where the map $\varphi : \mathcal{A} \to \mathbb{R}^3$ defines the position of the mid-surface of the shell, and the map $\mathbf{t} : \mathcal{A} \to S^2$ defines a unit vector field as the director field.

*J.C. Simo, D.D. Fox [1989], On a stress resultant geometrically exact shell model. Part I : Formulation and optimal parameterization. *Comput. Methods Appl. Mech. Engrg.* 72(3), 267-304.

Let $\{\mathbf{E}_i\}_{i=1,2,3}$ an orthonormal basis as the standard basis. Then $\mathbf{t}$ may be defined as $\mathbf{t} = \mathbf{\Lambda}\mathbf{E}_3$, where $\mathbf{\Lambda} \in S^2_{E_3}$, a $SO(3)$ *Lie subgroup*.

$S^2_{E_3} := \{\mathbf{\Lambda} \in SO(3) |\, \forall\, \Psi \in \mathbb{R}^3$ such that $\mathbf{\Lambda}\Psi = \Psi$, then $< \Psi, \mathbf{E}_3 >= 0\}$

And the time differentiation of the director $\mathbf{t}$ is

$$\dot{\mathbf{t}} = \dot{\mathbf{\Lambda}}\mathbf{E} = \mathbf{\Lambda}\widehat{\mathbf{W}}\mathbf{E}$$

where $\dot{\mathbf{t}} \in TS^2$, and $\widehat{\mathbf{W}} \in T_1 S^2_{E_3} \subset \mathfrak{so}(3)$, where $\widehat{\mathbf{W}}$ represents an infinitesimal rotation about $\mathbf{W} \in \mathbb{R}^3$ define as follows :

$\mathfrak{so}(3)$ may be identified with $\mathbb{R}^3$ by the isomorphism

$$\widehat{\ } : \mathbb{R}^3 \rightarrow \mathfrak{so}(3), \quad \mathbf{W} = (W_1, W_2, W_3) \mapsto \widehat{\mathbf{W}} = \begin{pmatrix} 0 & -W_3 & W_2 \\ W_3 & 0 & -W_1 \\ -W_2 & W_1 & 0 \end{pmatrix}$$

with the identity $\widehat{\mathbf{W}}\mathbf{V} = \mathbf{W} \times \mathbf{V}$, for all $V \in \mathbb{R}^3$. $\square$

Hamiltonian Noether's theorem. When the Lie group action is a symmetry group of the Hamiltonian, then the corresponding Hamiltonian momentum maps $\mathbf{J} : T^*Q \to \mathfrak{g}^*$ are preserved by the Hamiltonian flow ϕ_t, that is $\mathbf{J} \circ \phi_t = \mathbf{J}$.

We have an **equivalent Lagrangian form of Noether's theorem**.

Examples : a) **Linear momentum**. Let the N-particles system and consider the translation on every factor, or $\mathbb{R}^3$-action on $\mathbb{R}^{3N}$. The total linear momentum of the N-particle system is

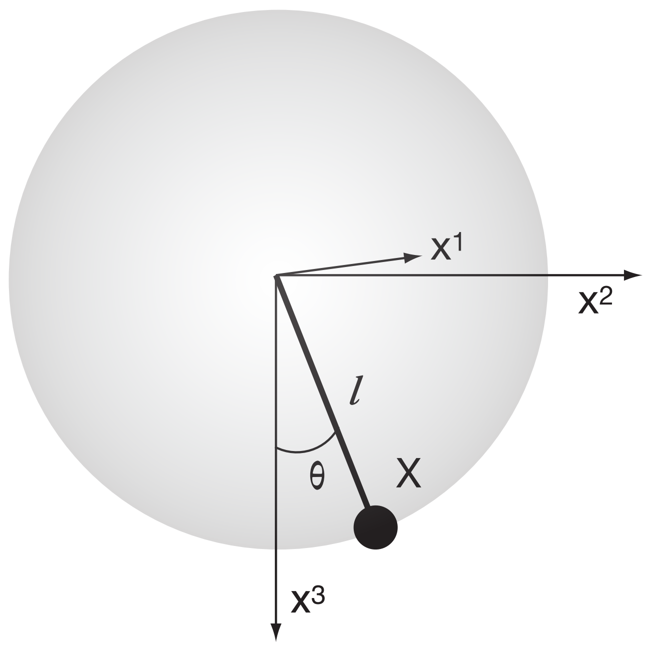
$$\mathbf{J}(\mathbf{q}_j, \mathbf{p}^j) = \sum_{j=1}^{N} \mathbf{p}^j$$

Given a Hamiltonian H, determining the evolution of the N-particle system, Noether's theorem establish that the total linear momentum $\mathbf{J}$ is conserved if H is translation-invariant.

b) **Angular momentum**. Let the symmetry group of the *pendulum* $G \subset SO(3)$ which acts on the configuration space $Q = S_l^2$. The angular momentum associated to one element of configuration space of the pendulum system is

$$\mathbf{J}(\mathbf{q}, \mathbf{p}) = \mathbf{q} \times \mathbf{p}$$

And in this case, Noether's theorem states that a Hamiltonian that is G-invariant has the three components of $\mathbf{J}$ as constants of the motion.



$\square$

Discrete mechanics

References for discrete mechanics

Jerrold E. Marsden, M. West [2001], Discrete mechanics and variational integrators. *Cambridge University Press*

Melvin Leok [2004], Foundations of computational geometric mechanics. *Thesis - Caltech*

M. West [2004], Variational integrators. *Thesis - Caltech*

Discrete mechanics

- a) Discrete variational mechanics
- b) Hamiltonian viewpoint
- c) One-step integrator and its properties
- d) Non-holonomic constraint

Discrete variational mechanics. Let a configuration manifold Q, as previously, but now define the **discrete state space** to be $Q \times Q$ (which contains the same amount of information as TQ).

To relate discrete to continuous mechanics, we introduce **sequence of time** $\{t_k = kh \mid k = 0, ..., N\}$, where $h \in \mathbb{R}$ is a **discrete time step**.

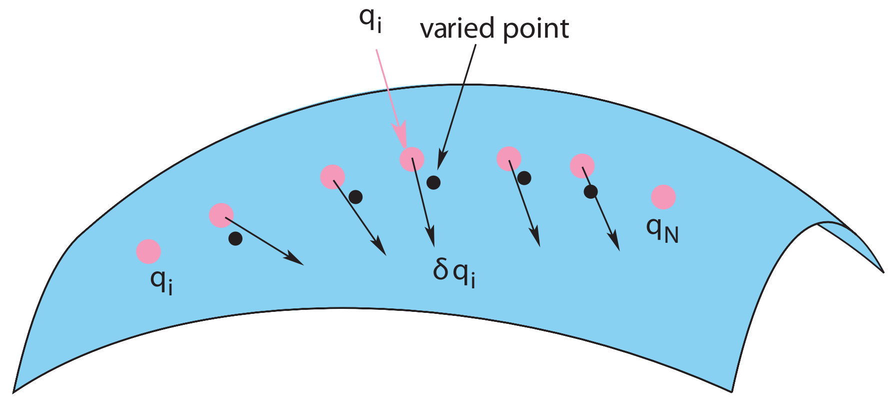
We can define the **discrete path space** $\mathcal{C}_d(Q) = \{\mathbf{q}_d : \{t_k\}_{k=0}^N \to Q\} = \{q_k\}_{k=0}^N$, which is isomorphic to $\mathbb{R} \times ... \times \mathbb{R}$, $(N+1$ copies), where $q_k = q(t_k)$.

The **discrete action map** $\mathfrak{S}_d : \mathcal{C}_d(Q) \to \mathbb{R}$ is defined by

$$\mathfrak{S}_d(q_d) = \sum_{k=0}^{N-1} L_d(q_k, q_{k+1}).$$

By computing variation of this action sum, with boundary q_0 and q_N fixed, we obtain the discrete **discrete Euler-Lagrange equations**

$$D_2 L_d(\mathbf{q}_{k-1}, \mathbf{q}_k) + D_1 L_d(\mathbf{q}_k, \mathbf{q}_{k+1}) = 0, \quad \text{for all} \quad k = 1, ..., N-1$$



If we take initial conditions $(\mathbf{q}_0, \mathbf{q}_1)$ then the discrete Euler-Lagrange equations define a recursive rule for calculating the sequence $\{\mathbf{q}_k\}_{k=0}^N$. We get a **variational integrator**

$$F_{L_d} : (\mathbf{q}_{k-1}, \mathbf{q}_k) \to (\mathbf{q}_k, \mathbf{q}_{k+1})$$

$L_d : Q \times Q \to \mathbb{R}$ is a **discrete Lagrangian of order $\mathbf{r}$**, if it satisfies

$$L_d(\mathbf{q}_k, \mathbf{q}_{k+1}, \Delta t) = \int_{t_k}^{t_{k+1}} L(q, \dot{\mathbf{q}}) dt + \mathcal{O}(\Delta t)^{r+1},$$

where L is the Lagrangian of the continuous systems and $\mathbf{q}(t)$ is the solution of the Euler-Lagrange equations satisfying $\mathbf{q}(t_k) = \mathbf{q}_k$ and $\mathbf{q}(t_{k+1}) = \mathbf{q}_{k+1}$.

Example : If we take, as discrete Lagrangian

$$L_d^{\alpha}(\mathbf{q}_k, \mathbf{q}_{k+1}, h) = hL\left((1-\alpha)\mathbf{q}_k + \alpha \mathbf{q}_{k+1}, \frac{\mathbf{q}_{k+1} - \mathbf{q}_k}{h}\right),$$

variational integrator is explicit for $\alpha = 0$ or $\alpha = 1$, but only first order. And is second order if and only if $\alpha = 1/2$, but in this case variational integrator is implicit.

An interesting choice of discrete Lagrangian is Lagrangian as kinetic energy minus potential energy, with $\alpha = 0$, to get explicit integrator

$$L_d(\mathbf{q}_k, \mathbf{q}_{k+1}, h) = \frac{h}{2}\left(\frac{\mathbf{q}_{k+1} - \mathbf{q}_k}{h}\right)^T M \left(\frac{\mathbf{q}_{k+1} - \mathbf{q}_k}{h}\right) - hV(\mathbf{q}_k). \quad \square$$

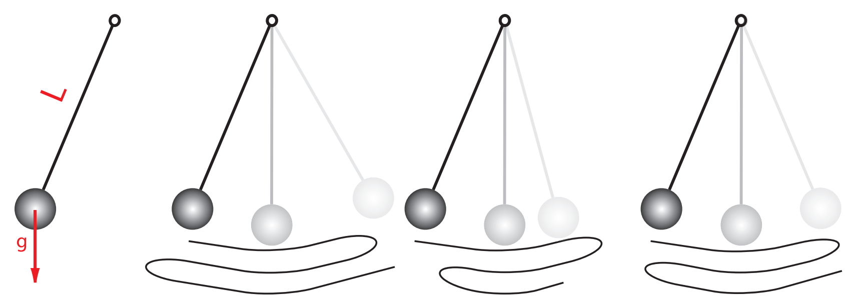
Hamiltonian viewpoint. Similarly to the definition of Legendre transform in continuous mechanics, we specify a discrete Legendre transform $\mathbb{F}^{\pm}L_d$, to relate discrete Lagrangian mechanics to Hamiltonian mechanics, in such a way that $\mathbb{F}^{\pm}L_d : Q \times Q \to T^*Q$ is defined as the derivative of L_d at (q_k, q_{k+1}) along $Q \times Q$, in two directions $\delta q_k \in T_{q_k}Q$ and $\delta q_{k+1} \in T_{q_{k+1}}Q$, so that the discrete Legendre transforme applied to $\left(q_k, q_{k+1}\right) \in Q \times Q$ has the expression

$$\left\{ \begin{array}{l} \mathbb{F}^{+}L_d\left(q_k, q_{k+1}\right) = \left(q_{k+1}, D_2 L_d\left(q_k, q_{k+1}\right)\right) \\ \mathbb{F}^{-}L_d\left(q_k, q_{k+1}\right) = \left(q_k, -D_1 L_d\left(q_k, q_{k+1}\right)\right) \end{array} \right. \tag{1}$$

Which allow us to establish a link between Lagrangian approximation and discrete Hamiltonien map when the Lagrangian L is regular, that is to say a strong link between variational integrators and symplectic integrators traditionally approached from Hamilton viewpoint (see Hairer, Lubich, Wanner (2002)).

Properties of one-step integrator : $F_{L_d} : (x_{k-1}, x_k) \mapsto (x_k, x_{k+1})$
It has two important structure preserving properties, as in continuous mechanics :

• First, F_{L_d} is **symplectic** which implies area preservation in phase-space or, more precisely, $\left(F_{L_d}\right)^* \Omega_{L_d} = \Omega_{L_d}$, where Ω_{L_d} is a discrete Lagrangian 2-form.



• Secondly, if discrete Lagrangian L_d inherits the same symmetry groups as the continuous system, which means it is invariant under a Lie group action, then the **discrete Lagrangian momentum map** J_{L_d} is a conserved quantity : $J_{L_d} \circ F_{L_d} = J_{L_d}$.

Non-holonomic constraint. Given **discrete Lagrangian forces** (which are fibre-preserving), we modify the discrete Hamiltons principle to the **discrete Lagrange-d'Alembert principle** which states that the discrete trajectory $\{q_k\}$, with prescribed initial and final endpoints, satisfy

$$\delta \sum_{k=0}^{N} L_d(q_k, q_{k+1}) + \sum_{k=0}^{N} \left[f_d^-(q_k, q_{k+1}) \delta q_k + f_d^+(q_k, q_{k+1}) \delta q_{k+1} \right] = 0$$

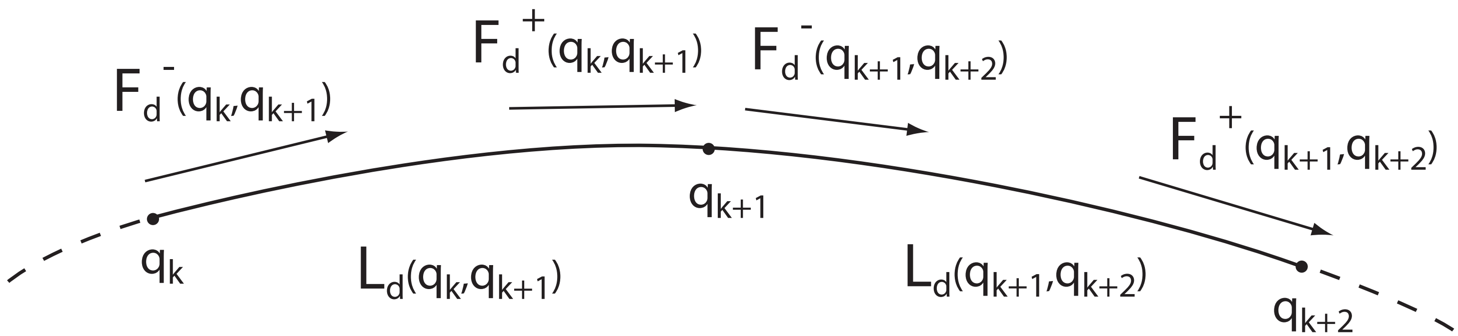
where f_d^- and f_d^+ are left and right discrete Lagrangian forces. And we get the **forced discrete Euler-Lagrange equations**

$$D_2 L_d (q_{k-1}, q_k) + D_1 L_d \left(q_k, q_{k+1} \right) + f_d^+ (q_{k-1}, q_k) + f_d^- \left(q_k, q_{k+1} \right) = 0,$$

The **forced discrete Lagrangian flow** $F_{L_d} : Q \times Q \to Q \times Q$, we get, is a one-step integrator, which conserve momentums associated to symmetries.

Example of Lagrangian discrete force

$$\begin{cases} f_d^-(q_k, q_{k+1}) = 0 \\ f_d^+(q_k, q_{k+1}) = -\lambda \frac{(q_{k+1}-q_k)}{(t_{k+1}-t_k)}, \qquad \lambda \in \mathbb{R} \end{cases}$$



AVI

References for AVI

A. Lew, J. E. Marsden, M. Ortiz, and M. West - Variational time integrators - International journal for numerical methods in engineering. 2003

J.E. Marsden, and M. West - Discrete mechanics and variational integrators - Cambridge University Press - 2001

AVI

- a) AVI and energy conservation.

- b) Convergence

- c) Simplicity and Noether's theorem for AVI

Conservation of energy. In order to achieve conservation of energy we also consider the time interval $[0, T]$ and define the **extended configurations** by $\tilde{\varphi} : \tilde{\mathcal{B}} \to \tilde{\mathcal{S}}$, with $\tilde{\mathcal{B}} := \mathbf{R} \times \mathcal{B}$, and $\tilde{\mathcal{S}} := \mathbf{R} \times \mathcal{S}$, where $\mathbf{R}$ is time axis.

We request the discrete action sum to be stationary with respect to variations both of the coordinates q_k and the time t_k. The resulting discrete Euler-Lagrange equations are

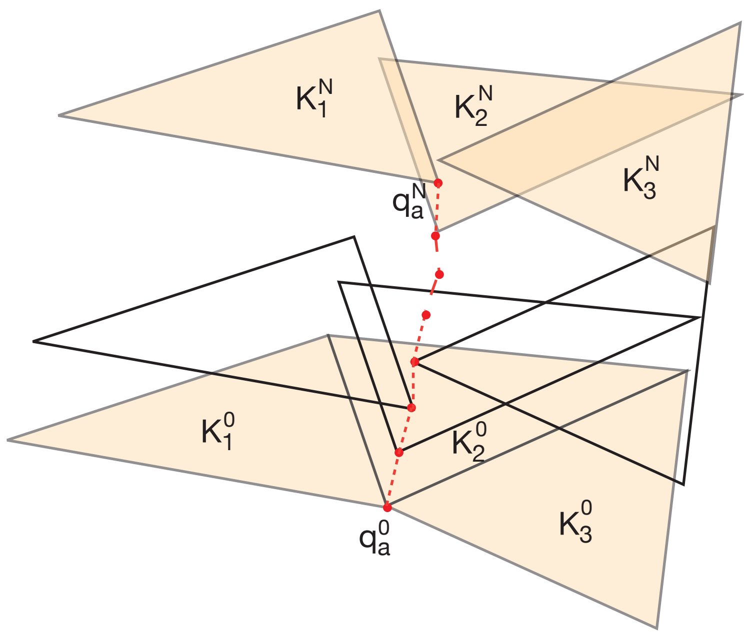
$$\begin{cases} D_2 L_d(\mathbf{q}_{k-1}, \mathbf{q}_k, t_k - t_{k-1}) + D_1 L_d(\mathbf{q}_k, \mathbf{q}_{k+1}, t_{k+1} - t_k) = 0 \\ \\ D_3 L_d(\mathbf{q}_{k-1}, \mathbf{q}_k, t_k - t_{k-1}) - D_3 L_d(\mathbf{q}_k, \mathbf{q}_{k+1}, t_{k+1} - t_k) = 0 \end{cases}$$

The first expression was already seen as variational integrator, and the second expresses the conservation of energy-momentum tensor, giving the value of the time step $t_{k+1} - t_k$ for each k. This new variational integrator, *with a particular implementation*, is now said to be an **Asynchronous Variational Integrator (AVI)**.

Example : Particles $\{a^i\}$ in subsystems $\{K^j\}$. The AVI composed by discrete Euler-Lagrange equations is satisfied by solving for both the coordinates $\mathbf{q}_a^i$ and the times t_K^j

$$\begin{cases} D_a^i \mathfrak{S}_d = 0 \\ D_K^j \mathfrak{S}_d = 0 \end{cases}$$

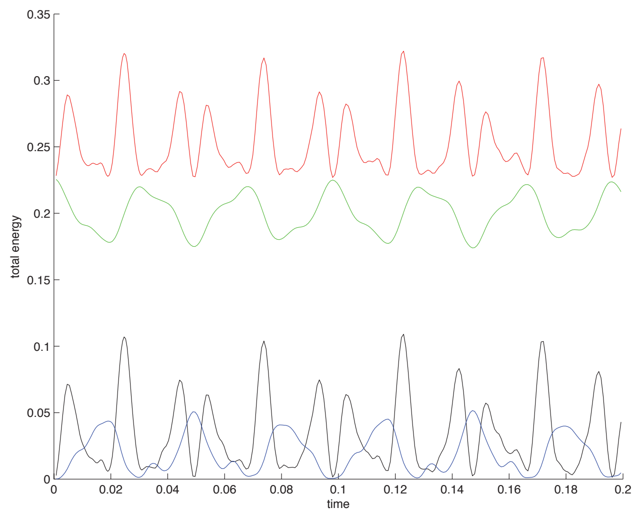
where we consider the discrete action sum as a function of the coordinates $\mathbf{q}_a^i$ of each particle a and the time t_K^j of each subsystem K. In other words, we restrict the time component t_a^i to coincide with the time t_K^j of one of the subsystem K.



$\square$

AVI allow different time steps at different points which is important for efficiency. However, *the implicit algorithm* $D_K^j \mathfrak{S}_d = 0$ *is not always very easy to calculate*. Fortunately, the total energy oscillates around a constant value for very long time without overall growth or decay, if we choose a particular time step for each cell, in relation both with the geometry of the mesh, and with material properties.

Example : Evolution over time of the total energy of a thin-shell being vibrate



green = exterior potential energy, **blue** = elastic potential energy, **black** = kinetic energy, **red** = total energy. $\square$

Example : Given the discrete Lagrangian

$$L_d(\mathbf{x}_k, \mathbf{x}_{k+1}, h) = h\left(\frac{1}{2}\left(\frac{\mathbf{x}_{k+1}-\mathbf{x}_k}{h}\right)^T M\left(\frac{\mathbf{x}_{k+1}-\mathbf{x}_k}{h}\right) - V(\mathbf{x}_k)\right),$$

where M is a symmetric, positive definite matrix, and $\{\mathbf{x}_k\}$ are vector positions in $\mathbb{R}^n$.

Let the **triangulation** $\mathcal{T}$ of $\mathcal{B}$ be composed of cells K with nodes a of mass $m_{a,K}$ such that $\sum_{a\in K} m_{a,K} = M_K$, where M_K is the mass of K. The vector positions of K and a at times t_K^j and t_a^i are denoted by $\mathbf{x}_K^j$ and $\mathbf{x}_a^i$.

We get an explicit **one-step integrator** giving the discrete speed v_a^i of node a, at time $t_a^i = t_K^j$

$$m_a\left(\frac{\mathbf{x}_a^{i+1}-\mathbf{x}_a^i}{t_a^{i+1}-t_a^i}\right) = m_a\left(\frac{\mathbf{x}_a^i-\mathbf{x}_a^{i-1}}{t_a^i-t_a^{i-1}}\right) - h_K\frac{\partial V_K}{\partial \mathbf{x}_K^j}(\mathbf{x}_K^j). \quad \square$$

Convergence of the AVI is known for time steps vanishing toward zero, for fixed spatial discretization.

Define the **maximum time step** and the **maximum final time**

$$\Delta t_{max} = \max_K (\Delta t_K), \quad t_{max} = \max_K (N_K \Delta t_K)$$

Lemma. Consider a sequence of solutions obtained by the application of asynchronous variational integrators, to a fixed spatial discretization, with maximum time step $\Delta t_{max} \to 0$ and maximum final time $t_{max} \to T$. Then the final discrete configuration converges to the exact solution at time T.

Remark. Even for corse mesh we get convergence.

Discrete simplicity, and discrete Noether's theorem for AVI.

One of the powerful features of variational multisymplectic discretization is that there is a unique discrete multisymplectic structure, as well as a **discrete multisymplectic Lagrangian two-forms** Ω_{L_d}.

And the discrete integrator F_{L_d} associated to AVI is **time-symplectic**

$$\Omega_{L_d} = \left(F_{L_d}\right)^* \Omega_{L_d}$$

In the same way it is always possible to define a **Noether's theorem for multisymplectic discretization**. And so on discrete symmetries of system are conserved.

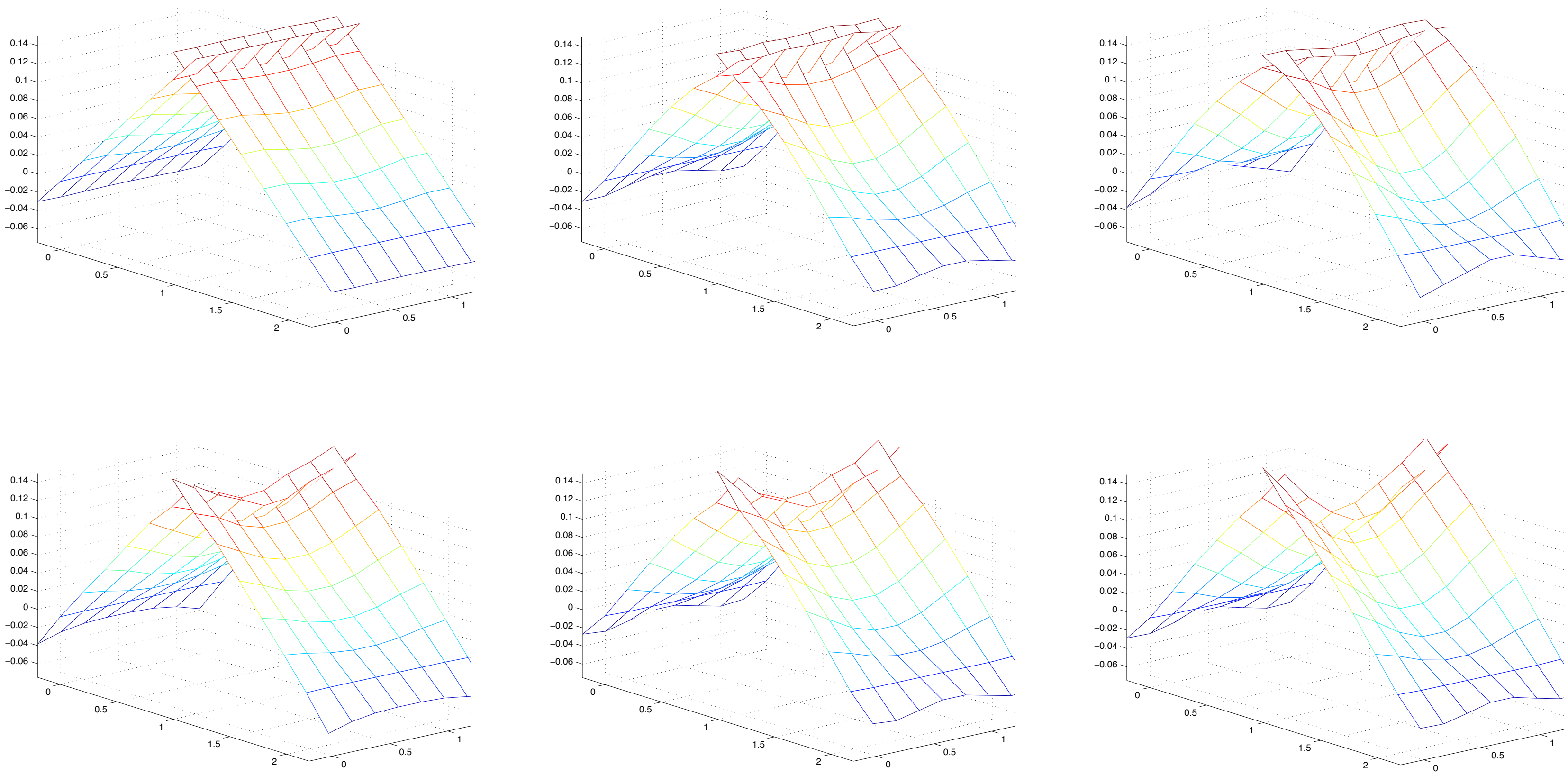
In conclusion AVI is a particular example of multisymplectic discretization where we get the same properties as with variational integrators, but we add conservation of energy, and the time step is adapted to each elements K of the mesh τ with great advantages, among all with complex systems described by different potential energy V_K according to sets of elements K. As the discrete action sum is

$$\mathfrak{S}_d = \sum_a \sum_{i=0}^{N_a-1} \frac{1}{2} m_a \left(t_a^{i+1} - t_a^i\right) \left\| \frac{x_a^{i+1} - x_a^i}{t_a^{i+1} - t_a^i} \right\| -$$

$$\sum_{K \in \tau} \sum_{j=0}^{N_K-1} \left(t_K^{j+1} - t_K^j\right) V_K \left(x_K^{j+1}\right)$$

where nodes a are associated to elements K, composed of different Lagrangian, we can adapt the time step to the size of the mesh and to Lagrangian's. And what it remains is to describe correctly mechanic phenomena of the system to study as in the next example.

Example : dynamics of thin-shells set, based on Kirchhoff-Love constraints



The advantage of these discrete variational integrators is that they preserve the symplectic structure (a classical property of mechanical systems), and preserve momenta for systems with symmetry, have excellent energy behavior (even with some dissipation added), and allow the usage of different time steps at different points. These properties significantly enhance the efficiency of these algorithms.